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Extended Watson Integral について

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積分

$$I_s(a; l, m, n) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\cos lx \cos my \cos nz dx dy dz}{a + i\epsilon - \cos x - \cos y - \cos z} \quad (0)$$

(ϵ は正の無限小) を考える。(0) は単純立方格子に対する

Green 関数であり、格子振動の振動数分布、強磁性の Heisenberg 模型、其他多くの物性物理学上の応用をもつ積分である。体心立方格子、面心立方格子に対しては

$$I_b(a; l, m, n) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\cos 2lx \cos 2my \cos 2nz dx dy dz}{a + i\epsilon - \cos x \cos y \cos z}$$

$$I_f(a; l, m, n) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\cos 2lx \cos 2my \cos 2nz dx dy dz}{a + i\epsilon - \cos x \cos y - \cos y \cos z - \cos z \cos x}$$

という積分があらわれるが、こゝでは $l = m = n = 0$ の場合の單

純立方格子を問題とする。

$I_s(3, 0, 0, 0)$, $I_b(1; 0, 0, 0)$, $I_f(3; 0, 0, 0)$ は Watson¹⁾ により求められ、居りその巧妙さには $\delta \approx 2(0)$ に Extended Watson Integral の名が冠せられた。

$I_s(a; 0, 0, 0)$ は $a > 3$ に対し実数。 $0 < a < 3$ に対しは複素数で $a=1$ と $a=3$ が特異点^{係数の値} となる。 $I_s(a > 3, 0, 0, 0)$ の $1/a^2$ による展開^{係数の値} は Tickson²⁾ により求められ、 $a > 3$ に対する数表が与えられた。

Maradudin, Montroll³⁾ 等は $I_s(a > 3; l, m, n)$ の $(a-3)$ による展開^{係数の最初の数項} を求め $a=3$ ($a > 3$) における leading term が $O((a-3)^{1/2})$ であることを示し、 $I_s(a > 3; l, m, n)$ の数表を与えた。 Mannari and Kawabata⁴⁾ は $I_s(a > 3; 0, 0, 0)$, $I_b(a > 1; 0, 0, 0)$, $I_f(a > 3; 0, 0, 0)$ を楕円積分およびその変形^{変形} であらわし、数値積分により詳細な数表を与えた。 Yussouff and Mahanty⁵⁾ は後述の(2)の実数部および虚数部を個々に Simpson 法で数値積分することにより、また Vashishta and Yussouff⁶⁾ は Fourier 級数による展開により $I_s(a; l, m, n)$, $I_b(a; l, m, n)$, $I_f(a; l, m, n)$ の数表を与えたが Ref. 5 と Ref. 6 との結果の差も

大きく相対誤差は 10~20% に達する所もあると思われる。

本積分は応用上多大の興味が持たれているに拘らず²⁾ 解析的及び数値的に知られていることは十分ではない。本論文 第1部では $I_S(a; 0, 0, 0)$ を Mellin-Barnes 型積分に変換し、その解析接続により $a > 3$ (real part) 及び $0 < a < 1$ (real part 及び imaginary part) の級数表示を求める方法をのべる。 $1 < a < 3$ については 第3部以下にゆずる。第2部においては $I_S(a; 0, 0, 0)$ が $0 < a < 1$, $1 < a < 3$ の場合にも楕円積分の定積分で表えられることを示し、これにより $I_S(a)$ を計算する。第1部の方法は関数の解析的性質が見易いこと、分子は ω のべき乗の項のある一般形式に拡張し易いことの特徴を有し、第2部の方法は 体心立方格子、面心立方格子に拡張し易いという特徴を有する。これ等については 第3部 以下にのべる予定である。

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Extended Watson Integral

Part I

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$$I(a) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dx dy dz}{a + i\epsilon - \cos x - \cos y - \cos z} \quad (1)$$

(1)は

$$= -\frac{i}{\pi^3} \int_0^\infty dt \int_0^\pi dx \int_0^\pi dy \int_0^\pi dz \quad \times \ell$$

$$i [(a + i\epsilon) - \cos x - \cos y - \cos z] t$$

と書ける. $\int_0^\pi dx \int_0^\pi dy \int_0^\pi dz$ を先に'行なうと

$$= -i \int_0^\infty e^{i(a+i\epsilon)t} [J_0(t)]^3 dt \quad (2)$$

Mellin-Barnes 型

$[J_0(t)]^2$ の級数表示を積分表示に持ち直すと

$$[J_0(t)]^2 = \sum_{m=0}^{\infty} \frac{(-)^m \left(\frac{t}{2}\right)^{2m} (m+1)_m}{m! [\Gamma(m+1)]^2}$$

$$= \frac{1}{\sqrt{\pi}} \frac{1}{2\pi i} \int_C ds \frac{\Gamma(-s) \Gamma(s + \frac{1}{2}) t^{2s}}{[\Gamma(s+1)]^2} \quad (3)$$

C は $s = -\Delta$ ($\Delta \rightarrow +0$) を通る虚軸に平行な直線である. (3) を (2) に入れ ds と dt の順序を交換すると

$$I(a) = \frac{-i}{\sqrt{\pi}} \frac{1}{2\pi i} \int_C ds \frac{\Gamma(-s) \Gamma(s + \frac{1}{2})}{[\Gamma(s+1)]^2}$$

$$\times \int_0^\infty e^{i(a+ie)t} J_0(t) t^{2s} dt \quad (4)$$

$\int_0^\infty dt$ は $\epsilon > 0$, $2s+1 > 0$ ならば収束して

$$\int_0^\infty dt = \frac{\Gamma(2s+1)}{(-ia)^{2s+1}} {}_2F_1\left(s+\frac{1}{2}, s+1; 1; \frac{1}{a^2}\right)$$

故に

$$I(a) = \frac{1}{\pi a} \frac{1}{2\pi i} \int ds \frac{\Gamma(-s) [\Gamma(s+\frac{1}{2})]^2}{\Gamma(s+1)} \left(-\frac{4}{a^2}\right)^s \times {}_2F_1\left(s+\frac{1}{2}, s+1; 1; \frac{1}{a^2}\right) \quad (5)$$

$|a| > 1$ ならば ${}_2F_1$ をそのまま展開して積分と総和の順序を変更すると

$$I(a) = \frac{1}{\pi a} \sum_{n=0}^{\infty} \frac{1}{n! \Gamma(1+n)} \left(\frac{1}{a^2}\right)^n \times \frac{1}{2\pi i} \int ds \left(-\frac{4}{a^2}\right)^s \frac{\Gamma(-s) \Gamma(s+\frac{1}{2}) \Gamma(s+\frac{1}{2}+n) \Gamma(s+1+n)}{[\Gamma(s+1)]^2} \quad (6)$$

$|a| > 2$ ならば積分路を右半面に閉じる。このとき被積分関数の極は $s=0, 1, 2, \dots, m, \dots$ であるから

$$I(a) = \frac{1}{\pi a} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{1}{2}) \Gamma(m+n+\frac{1}{2}) \Gamma(m+n+1) 4^m}{n! \Gamma(1+n) m! [\Gamma(1+m)]^2} \left(\frac{1}{a^2}\right)^{m+n} \quad (7)$$

(7) を一般化して 2 重級数

$$I(x, y) = \frac{1}{\pi a} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{1}{2}) \Gamma(m+n+\frac{1}{2}) \Gamma(m+n+1)}{n! \Gamma(n+1) m! [\Gamma(t+m)]^2} 4^m x^m y^n$$

$$\equiv \sum_n \sum_m A_{mn} x^m y^n \quad (8)$$

の収束域をしらべて見る. $m = t\mu$, $n = t\nu$ とおくと

$$\frac{1}{r} \equiv \lim_{t \rightarrow \infty} \frac{A_{m+1, n}}{A_{mn}} = \frac{4(\mu+\nu)^2}{\mu^2}$$

$$\frac{1}{s} \equiv \lim_{t \rightarrow \infty} \frac{A_{m, n+1}}{A_{mn}} = \frac{(\mu+\nu)^2}{\nu^2}$$

より

$$4r + s + \sqrt{16rs} = 1 \quad (9)$$

$r = s$ とおくと $r = \frac{1}{9}$ となる. 即ち (7) は $a > 3$ で収束する. $m+n=p$ とおくと (7) は

$$I(a) = \frac{1}{\pi a} \sum_{p=0}^{\infty} \Gamma(p+\frac{1}{2}) \Gamma(p+1) \left(\frac{1}{a^2}\right)^p$$

$$\times \sum_{m=0}^p \frac{\Gamma(m+\frac{1}{2}) 4^m}{(m!)^3 [(p-m)!]^2} \quad (10)$$

これは

となる. $\left(\frac{1}{a^2}\right)$ のべき級数で $\left(\frac{1}{a^2}\right)^p$ の係数は有限級数である.

数値計算には (10) を用いる. $a > 3$ では虚数部は消える.

(7)は a が大きい場合の展開であつたが積分表示 (5) を解析接続することにより a が小さい場合の展開を求めよう. 超幾何関数の変換公式により ${}_2F_1(\ ;\ ; 1/a^2)$ を ${}_2F_1(\ ;\ ; a^2)$ にかゝると

$$I(a) = \frac{1}{\pi a} \frac{1}{2\pi i} \int ds \frac{\Gamma(-s) [\Gamma(s+\frac{1}{2})]^2}{\Gamma(s+1)} \left(-\frac{4}{a^2}\right)^s$$

$$\times \left[\frac{\Gamma(\frac{1}{2})}{\Gamma(s+1)\Gamma(-s+\frac{1}{2})} \left(-\frac{1}{a^2}\right)^{-s-\frac{1}{2}} {}_2F_1\left(s+\frac{1}{2}, s+\frac{1}{2}; \frac{1}{2}; a^2\right) \right.$$

$$\left. + \frac{\Gamma(-\frac{1}{2})}{\Gamma(s+\frac{1}{2})\Gamma(-s)} \left(-\frac{1}{a^2}\right)^{-s-1} {}_2F_1\left(s+1, s+1; \frac{3}{2}; a^2\right) \right] \quad (11)$$

[] 内第1項は imaginary part, 第2項は real part を示す. これを $I(a) = I_R(a) + I_I(a)$ と記すこととする.

Real part: (11) の第2項の ${}_2F_1$ を展開し級数の和と積分の順序を変更すると

$$I_R(a) = a \sum_{n=0}^{\infty} \frac{a^{2n}}{n! \Gamma(n+\frac{3}{2})}$$

$$\times \frac{1}{2\pi i} \int ds \frac{\Gamma(s+\frac{1}{2}) [\Gamma(s+1+n)]^2 4^s}{[\Gamma(s+1)]^3} \quad (12)$$

$\int ds$ の中が 4^s であるの2種類分路は左半円を閉じ
 なければならぬ。分子の pole は $s + \frac{1}{2} = 0, -1, -2, \dots$
 (simple pole) と $s + 1 + n = 0, -1, -2, \dots$ (double
 pole) であるが、後者は分母の pole により相殺さ
 れるから前者のみを考えればよい。留数を求めると

$$I_R(a) = \frac{a}{2\pi} \sum_n \sum_m \frac{[\Gamma(\frac{1}{2} + m)]^3 (\frac{1}{4})^m (a^2)^n}{n! m! \Gamma(\frac{3}{2} + n) [\Gamma(\frac{1}{2} - n + m)]^2} \quad (13)$$

(13) を一般化して $T_2 = \sum A_{mn} x^m y^n$ について
 収束域を求めると (9) を求めるときと同様に

$$\frac{1}{y} = \frac{\mu^2}{(\mu - \nu)^2}, \quad \frac{1}{s} = \frac{(\mu - \nu)^2}{\nu^2}$$

より

$$\frac{1}{\sqrt{y}} - \sqrt{s} = 1 \quad (14)$$

故に (13) は $x = \frac{1}{4}$ に於ては $y (= a^2) = 1$ から収束
 半径を定める。従って (13) は $a < 1$ で用いられる。

$a < 1$ における imaginary part : (11) の [] 内
 第1項の寄与は

$$I_I(a) = \frac{-i}{\sqrt{\pi}} \frac{1}{2\pi i} \int ds \, 4^s \frac{\Gamma(-s) [\Gamma(s + \frac{1}{2})]^2}{[\Gamma(s+1)]^2 \Gamma(-s + \frac{1}{2})} \\ \times {}_2F_1(s + \frac{1}{2}, s + \frac{1}{2}; \frac{1}{2}; a^2) \quad (15)$$

$${}_2F_1 \text{ 在 } a^2 \text{ 附近展开}$$

$$I_I(a) = -i \sum_{n=0}^{\infty} \frac{a^{2n}}{n! \Gamma(-\frac{1}{2} + n)} \frac{1}{2\pi i} \int ds \frac{\Gamma(-s) [\Gamma(s + n + \frac{1}{2})]^2}{[\Gamma(s + 1)]^2 \Gamma(-s + \frac{1}{2})} 4^s \quad (16)$$

積分路を左半面 $2''$ 周 $5''$ 回すれば $2''$ と $5''$. $S = -\frac{1}{2} - n - m$,
 $m = 0, 1, 2, \dots$ かつ double pole $2''$ あり、留数計算ありと

$$\begin{aligned}
& \frac{1}{2\pi i} \int ds \ 4^s \frac{\Gamma(-s) [\Gamma(s+n+\frac{1}{2})]^2}{[\Gamma(s+1)]^2 \Gamma(-s+\frac{1}{2})} \\
&= \sum_{m=0} \left[\frac{d}{ds} (s+\frac{1}{2}+n+m)^2 \frac{[\Gamma(s+n+\frac{1}{2})]^2 \Gamma(-s) 4^s}{[\Gamma(s+1)]^2 \Gamma(-s+\frac{1}{2})} \right]_{s=-\frac{1}{2}-n-m} \\
&= \sum_{m=0} \left[\frac{d}{ds} \frac{\pi^2 (s+\frac{1}{2}+n+m)^2}{\sin^2[\pi(-s-n-\frac{1}{2})]} \frac{\Gamma(-s) 4^s}{[\Gamma(1-s-n-\frac{1}{2})]^2 [\Gamma(s+1)]^2 \Gamma(-s+\frac{1}{2})} \right] \\
&= \sum_{m=0} \frac{\Gamma(\frac{1}{2}+m+n) 4^{-\frac{1}{2}-n-m}}{[\Gamma'(1+m)]^2 [\Gamma(\frac{1}{2}-m-n)]^2 \Gamma(1+n+m)} \\
&\quad \times \left\{ -\psi(\frac{1}{2}+m+n) + 2\psi(1+m) - 2\psi(\frac{1}{2}-m-n) + \psi(1+n+m) \right. \\
&\quad \left. + \log 4 \right\} \tag{17}
\end{aligned}$$

故 12

$$I_I(a) = i \frac{1}{2\pi^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\left(\frac{a^2}{2^2}\right)^n \left(\frac{1}{4}\right)^m \left[\Gamma\left(\frac{1}{2} + m + n\right)\right]^3}{n! \Gamma\left(\frac{1}{2} + n\right) [\Gamma(1+m)]^2 \Gamma(1+m+n)} \\ \times \left\{ 3\psi\left(\frac{1}{2} + m + n\right) - 2\psi(1+m) - \psi(1+n+m) - \log 4 \right\} \quad (18)$$

(18) の収束半径も $a < 1$ である。

$I_R(a)$ の $a=1$ における値は正確に求めることが出来る。すなわち (13) より \sum_m を先に行くと

$$I_R(a) = \frac{a}{\pi^{3/2}} \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{1}{2})}{m!} \left(\frac{1}{4}\right)^m {}_2F_1\left(\frac{1}{2}-m, \frac{1}{2}-m; \frac{3}{2}; a^2\right)$$

$a=1$ を入れ ${}_2F_1(\quad; \quad; 1)$ の公式を用いると

$$I_R(1) = \frac{\Gamma(\frac{3}{2})}{\pi^{3/2}} \sum_{m=0}^{\infty} \frac{(\frac{1}{4})^m \Gamma(\frac{1}{2}+m) \Gamma(\frac{1}{2}+2m)}{m! [\Gamma(1+m)]^2}$$

$\Gamma(\frac{1}{2}+2m)$ を倍角公式で分解すると \sum_m は ${}_3F_2$ と

なり、 ${}_3F_2(\quad; \quad; 1)$ の公式より

$$I_R(1) = \frac{\Gamma(\frac{1}{2}) \Gamma(\frac{1}{4}) \Gamma(\frac{3}{4})}{\pi^{3/2} 2^{3/2}} {}_3F_2\left(\frac{1}{4}, \frac{1}{2}, \frac{3}{4}; 1, 1; 1\right)$$

$$= \frac{\pi}{2} \frac{1}{[\Gamma(\frac{5}{8})]^2 [\Gamma(\frac{7}{8})]^2}$$

$$= 0.6428822$$

${}_2F_1(\quad; \quad; a^2)$ は ${}_2F_1(\quad; \quad; 1-a^2)$ および ${}_2F_2(\quad; \quad; 1-\frac{1}{a^2})$ に変換し得るからこれより $I_R(a)$ および $I_I(a)$ の $1-a^2$ に関する展開, $1-\frac{1}{a^2}$ に関する展開を求めることが出来る。前者は $a \leq 1$ で、後者は

は $1 \leq a < 3$ で用いることが出来る. 特にこれより

$$\frac{I_R(1)}{I_I(1)} = \frac{1}{8} \frac{[\Gamma(\frac{3}{4})]^2}{[\Gamma(\frac{7}{8})]^4} + \frac{1}{4} \frac{[\Gamma(\frac{1}{4})]^2}{[\Gamma(\frac{5}{8})]^4}$$

$$= 0.6428822$$

$$0.9091728$$

が得られる. 数値計算の結果とともに
 詳細については第3報以下にゆづる.

Extended Watson Integral. Part II.

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1. Introduction

In this paper we present numerical values of the integral:

$$G(s) = \frac{1}{\pi^3} \int_0^\pi dx \int_0^\pi dy \int_0^\pi dz \frac{1}{s + i\epsilon - \cos x - \cos y - \cos z} \quad (1)$$

where s takes on real values and ϵ is an infinitesimal positive number. Watson¹⁾ expressed the value for $s=3$ in terms of the complete elliptic integral of the first kind.

The function $G(s)$ has an imaginary part when $-3 < s < 3$. It is related with the level density of vibrational mode of harmonic simple cubic lattice. The function as a function of s was given in a number of works presented in the past.²⁾ But no table of the values is available.

The function $G(s)$ for $s > 3$ is real and appears when one considers the localized mode of oscillation when one defect is imbedded in a simple cubic harmonic lattice. A short table was given by Maradudin et al.³⁾ and a detailed table was presented by Mannari and Kawabata.⁴⁾ Moreover a Chebyshev interpolation formula was prepared by Mannari and Kageyama.⁵⁾

In evaluating $G(s)$ for $s > 3$, Mannari and Kawabata started with its expression $G(s) = G_R(s)$ where

$$G_R(s) = \frac{1}{\pi^2} \int_0^{\pi/2} dx \, k K(k), \quad (2)$$

where

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}}, \quad (3)$$

$$k = 2 / (s - \cos x). \quad (4)$$

This expression was obtained by introducing the variable θ by

$$\frac{2 - k(1 + \cos y)}{2 + k(1 - \cos y)} = \frac{1 - k^2 \sin^2 \theta}{1 + k} \quad (5)$$

after the integration over z . In the present paper, we consider the real as well as the imaginary part of $G(s)$ for $s < 3$. For each part, we introduce a variable θ by a relation similar to (5) and express the integral as an integral of the elliptic function, similar to (2). Then a numerical computation of the integral is attempted.

In §2, the formulas by which numerical calculation is performed are derived. The numerical calculation is discussed in §3.

2. Results of integration over z

The integration over z for fixed values of x and y is performed as usual. The result is real or pure imaginary according as the absolute value of

$$D \equiv s - \cos x - \cos y \quad (6)$$

is more or less than unity. More explicitly one has

$$G(s) = G_R(s) + i G_I(s), \quad (7)$$

$$G_R(s) = \frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{(s - \cos x - \cos y)^2 - 1}} \quad (s - \cos x - \cos y > 1) \\ - \frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{(s - \cos x - \cos y)^2 - 1}} \quad (s - \cos x - \cos y < -1) \quad (8)$$

and

$$G_I(s) = -\frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{1 - (s - \cos x - \cos y)^2}} \quad (-1 < s - \cos x - \cos y < 1) \quad (9)$$

It is straightforward to see that $G_R(s)$ is an odd function and $G_I(s)$ is an even function of s :

$$G_R(-s) = -G_R(s) \quad (10)$$

$$G_I(-s) = G_I(s) \quad (11)$$

Hence in the following we consider $G_R(s)$ and $G_I(s)$ only for positive s .

The expressions (8) and (9) are investigated separately for three cases of positive s :

$$\text{I: } 3 < s,$$

$$\text{II: } 1 < s < 3,$$

$$\text{III: } 0 < s < 1.$$

Case I.

For case I, there exist no region of integral for the integral (9) and the second integral of (8). The inequality $s - \cos x - \cos y > 1$ is satisfied for all values of x and y between 0 and π . Hence

$$G_R(s) = \frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{1}{\sqrt{(s - \cos x - \cos y)^2 - 1}}, \quad (12)$$

$$G_I(s) = 0 \quad (13)$$

By introducing k and θ by (4) and (5), one can write (12) as (2)-(4).

Case II.

In Fig. 1, the region of integral is shown by taking $\cos x$ and $\cos y$ as abscissa and ordinate. The integral is taken in the square restricted by the lines $\cos x = \pm 1$ and $\cos y = \pm 1$. The region is divided by the line $D \equiv s - \cos x - \cos y = 1$, which cuts the abscissa at $\cos x = s - 1$. For the present case $s - 1$ is between 0 and 2. In the right-top region, $-1 < D < 1$ and $G_I(s)$ has a contribution from this region. In the left-bottom region, $D > 1$ and the first terms of (8) is contributed from this region.

The second term of (8) is zero.

Fig. 1

In the evaluation of $G_I(s)$, the variable k_1 and θ are introduced by

$$k_1 = \frac{s - \cos x}{2} \quad (14)$$

$$\frac{-2k_1 + (1 + \cos y)}{2k_1 + (1 - \cos y)} = \frac{(1 - k_1) \cos^2 \theta}{k_1} \quad (15)$$

Then one finds

$$G_I(s) = -\frac{1}{\pi^2} \int_0^{\cos^{-1}(s-2)} dx K(k_2), \quad (16)$$

where

$$k_2 = \frac{1}{2} \sqrt{4 - (s - \cos x)^2} \quad (17)$$

In evaluating $G_R(s)$, one separates the region of integral by whether $\cos x$ is less or more than s . For the latter region, the variable k_1 and θ are introduced by (14) and

$$\frac{2k_1 - (1 + \cos y)}{2k_1 + (1 - \cos y)} = \frac{k_1 \cos^2 \theta}{1 + k_1} \quad (18)$$

For the latter region, k and θ introduced for the case I are used.

Then one gets

$$G_R(s) = \frac{1}{\pi^2} \int_0^{\cos^{-1}(s-2)} dx K(k_1) + \frac{1}{\pi^2} \int_{\cos^{-1}(s-2)}^{\pi} dx K(k), \quad (19)$$

where k is given by (4).

Case III.

The region of integral is shown in Fig. 2, where the lines $D=1$ and $D=-1$ are drawn. The region in between these two lines contributes to $G_I(s)$. This region is divided by whether $\cos x$ is more or less than s . For the former region, variable k'_1 and θ are introduced by

$$k'_1 = \frac{\cos x - s}{2} \equiv -k_1 \quad (20)$$

$$\frac{-2k'_1 + (1 - \cos y)}{2k'_1 + (1 + \cos y)} = \frac{(1 - k'_1) \cos^2 \theta}{k'_1} \quad (21)$$

The calculation for the former region is similar to the one for region II.

$G_I(s)$ obtained is summed up, giving the result:

$$G_I(s) = -\frac{1}{\pi^2} \int_0^{\pi} dx K(k_2) \quad (22)$$

where k_2 is given by (17).

Fig. 2

The right-top region is the region of integral for the second term of (8). For its evaluation, θ is introduced by

$$\frac{-2R'_1 + (1 - \cos y)}{-2R'_1 - (1 + \cos y)} = \frac{R'_1 \cos^2 \theta}{1 + R'_1}, \quad (23)$$

where k'_1 is given by (14). The left-bottom region is the region of integral for the first term of (8). Its evaluation is done in a similar way to the contribution of $G_R(s)$ from $s-2 < \cos x$ in the case II. The result we obtain is

$$G_R(s) = \frac{1}{\pi^2} \int_{\cos^{-1}s}^{\pi} dx K(k_1) - \frac{1}{\pi^2} \int_0^{\cos^{-1}s} dx K(k'_1), \quad (24)$$

where k_1 and k'_1 are given by (14) and (20), respectively.

3. Numerical calculation

The calculation of the functions $G_R(s)$ and $G_I(s)$ is performed with the aid of (16) and (19) for $1 < s < 3$ and (22) and (24) for $0 < s < 1$. The integration is performed by the Simpson formula. The complete elliptic function appearing in the integrand is evaluated by the method of arithmetic-geometric means.⁶⁾

For the b. c. c. and f. c. c. lattices, the corresponding formulas of calculating the real and imaginary parts of the extended Watson integral. The numerical calculation is in progress with the aid of the computer of the computer center of Tohoku University.

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Captions

Fig. 1. The regions of integrations (8) and (9) for $G_R(s)$ and $G_I(s)$, respectively, when $1 < s < 3$. The regions hatched by horizontal and vertical lines are for the integral (9) and the first term of (8), respectively. When $k=1$, $k_1=1$ also and both integrands of (19) for $G_R(s)$ are singular. The integrand of (16) for $G_I(s)$ is singular at $k_2=1$. The latter singularity is important only when $s \approx 1$.

Fig. 2. The regions of integrations (8) and (9) for $G_R(s)$ and $G_I(s)$, respectively, when $0 < s < 1$. The region hatched by horizontal lines is for (9). There are two regions hatched vertically. The right-top one is for the second term of (8) and the left-bottom region is for the first term. When $k_2=1$, the integrand of (22) for $G_I(s)$ is singular. Both integrands of (24) for $G_R(s)$ are singular at $k_1=1$ where $k'_1=1$ also. The latter singularity is important only when $s \approx 1$.

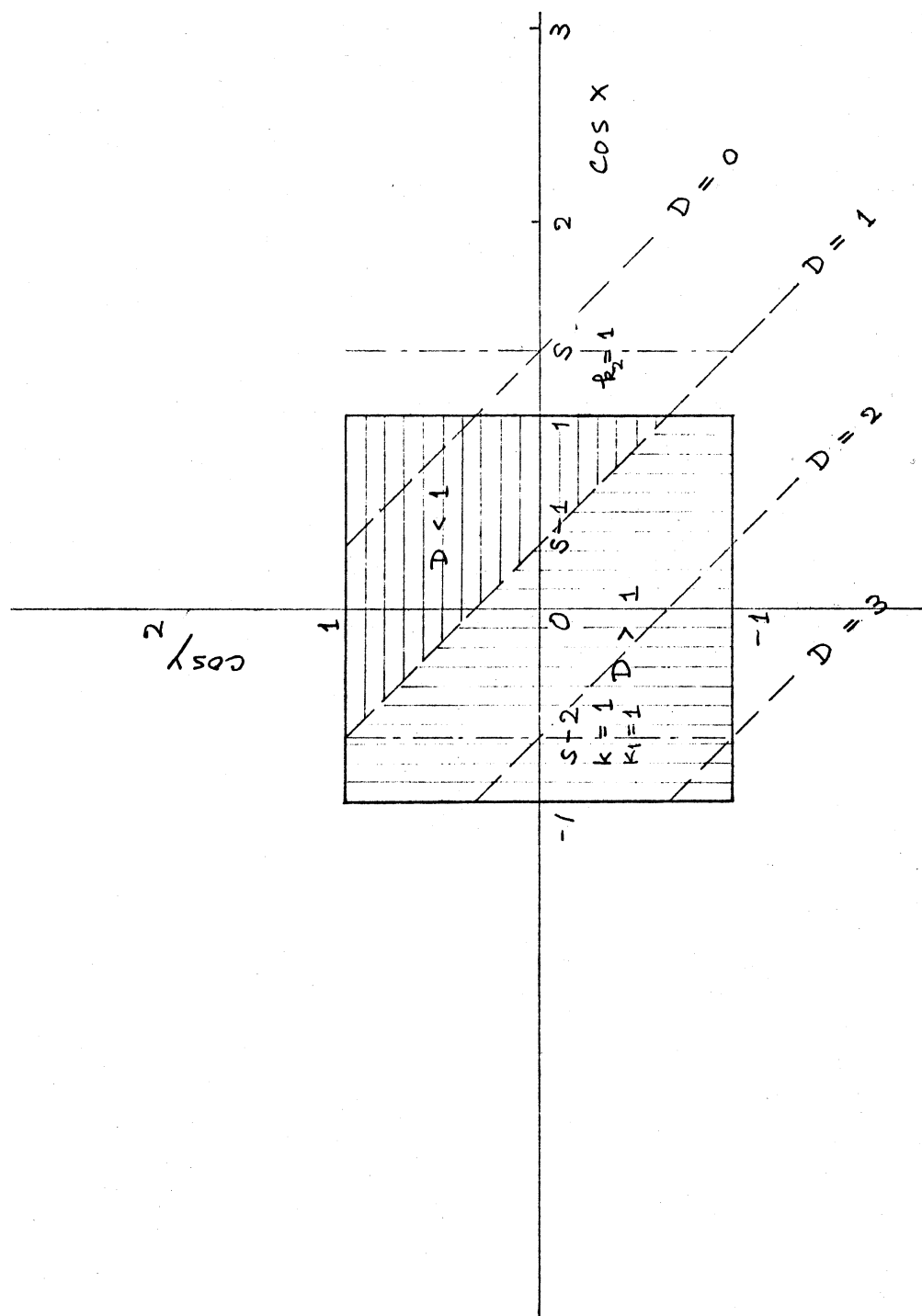


Fig. 1

